AD-A258 694

:NTATION PAGE

Form Approved
OMB No 0704-0188

ORT DATE

3 REPORT TYPE AND DATES COVERED
FINAL 1 Oct 90 - 31 Jan 92

2

4. TITLE AND SUBTITLE
"GEOMETRY OF ENERGY MINIMIZING SURFACES" (U)

5 FUNDING NUMBERS
6912/OR

6. AUTHOR(S)
Dr. Jean E. Taylor

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Rutgers-The State University
Department of Mathematics
Busch Campus
New Brunswick, NJ 08903

8. PERFORMING ORGANIZATION REPORT NUMBER

9 SPONSORING MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR/NM
Bldg 410
Bolling AFB DC 20332-6448

10 SPONSORING MONITORING AGENCY REPORT NUMBER
AFOSR-91-0010

DTIC
ELECTE
DEC 2 9 1992
S A D

11 SUPPLEMENTARY NOTES

12a DISTRIBUTION AVAILABILITY STATEMENT
Approved for public release;
Distribution unlimited

12b DISTRIBUTION CODE
UL

13 ABSTRACT (Maximum 200 words)

During this period of support they have continued long-term program of investigating the shapes of surfaces in mathematical models for crystals (including polycrystalline materials), both in equilibrium and in growth. The accomplishments included the completion of seven papers, all of which have either appeared in print or are in press, and working on five more, three of which have since been finished and accepted for publication. Also completed one videotape that will soon be published. Four papers that had previously been written appeared in print during the period of this grant. In addi- n, one AMA Special Session was organized and one week long workshop at The Geometry Center, and initiated and edited the proceedings of both (the second after this grant expired). These proceedings are highly innovative in that they include videotapes. The PI gave a large number of invited talks at a variety of meetings

14 SUBJECT TERMS	15. NUMBER OF PAGES 6
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18 SECURITY CLASSIFICATION OF THIS PAGE	19 SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	SAR

NSN 7540-01-280-5500

Standard Form 298 (Rev 2-89)
Prescribed by ANSI Std Z39-18
298-102

RUTGERS - THE STATE UNIVERSITY

FINAL REPORT FOR

AFOSR-91-0010

PROFESSOR JEAN E. TAYLOR

PERIOD OF PERFORMANCE

1 OCT 90 - 31 JAN 92

92-32899

92 ... 4

SENT BY:Xerox Telecopier 7020 ;11-24-92 ; 8:40AM ; 2019323257→ 202 404 7951;# 1

THE STATE UNIVERSITY OF NEW JERSEY
RUTGERS

Office of Research and Sponsored Programs
Administrative Services Building • Suite 123 • Busch Campus
P.O. Box 1089 • Piscataway • New Jersey 08855-1089
908/932-2880 • FAX 908/932-3257 • E-mail: U025001@RUTADMIN.BITNET

TELECOPIER TRANSMITTAL SHEET

SENDER's Telephone Number: (908) 932-2880

DATE: 11/24/92 Number of pages (including cover sheet) 6

TO: Elizabeth Coleman

FAX NUMBER: 202-404-7951

FROM: David A. Rumbo Contract/Grant Manager

SUBJECT: Final Report for AFOSR Grant 91-0010

MESSAGE: Please advise if anything futher is required.

Operator: [signature]

Accesion For	
NTIS CRA&I	☑
DTIC TAB	☐
Unannounced	☐
Justification	
By	
Distribution /	
Availability Codes	
Dist	Avail and / or Special
A-1	

FINAL TECHNICAL REPORT

for the period October 1 1990 - January 31 1992

Jean E. Taylor

During this period of support I continued my long-term program of investigating the shapes of surfaces in mathematical models for crystals (including polycrystalline materials), both in equilibrium and in growth. My accomplishments included the completion of seven papers, all of which have either appeared in print or are in press, and working on five more, three of which have since been finished and accepted for publication. I also completed one videotape which has been published and did part of the work which has since resulted in another videotape that will soon be published. Four papers that I had previously written appeared in print during the period of this grant. In addition I organized one AMS Special Session and one week-long workshop at The Geometry Center, and initiated and edited the proceedings of both (the second after this grant expired). These proceedings are highly innovative, in that they include videotapes. I also gave a large number of invited talks at a variety of meetings.

The surface energy of the interface of a crystal with some other given material, such as another crystal, or its melt or vapor or some other matrix, is a function of the oriented normal direction $\mathbf{n}$ of the interface. If this surface energy per unit area (i.e., surface tension) γ *is* sufficiently anisotropic, then the Wulff shape, which is the equilibrium shape of a single crystal surrounded by the other material, is a polyhedron; this is the *crystalline* case by definition, although not all physical crystals have surface tensions with completely facetted Wulff shapes. There are many other situations besides that of a single crystal in equilibrium in which surface energy plays a role: grain boundaries in a polycrystalline solid, analogs of minimal surfaces and of soap films on wire frames, and various types of crystal growth and dissolution.

In growth problems, another factor is the mobility M (also a function of the unit normal n), which is the ratio of the normal velocity to the force driving it to move (assuming a linear response to the driving force). The driving force can include both surface energy reduction and bulk energy reduction, due to a phase change; I have considered cases where the bulk energy part is zero, is constant, depends only on position and time, depends on the local shape of the surface, and depends on a diffusion field (like temperature or concentration).

My research accomplishments during this year included:

1. Writing three papers (one being the definitive research paper, the other two being relatively short expository papers about the results) and finishing a videotape on the motion of polycrystalline interfaces in 2-d in the crystalline case. Here the normal velocity of a segment S_i is of the form

$$-M(\mathbf{n}(S_i))(\Omega + wmc(S_i)),$$

where $\mathbf{n}(S_i)$ is the oriented unit normal of S_i, Ω is a constant, and *wmc* stands for "weighted mean curvature." *wmc* is defined to be the rate of decrease in surface energy with volume under deformations consisting of changing the distance of S_i from the origin while keeping

its same orientation and adjacencies to other segments. For a line segment in a crystalline polygonal curve in the plane, *wmc* turns out to be just the length of the segment on the boundary of the Wulff shape with the same normal, divided by the length of the segment in the polygonal curve, times 1, -1, or 0 (depending on whether the adjacent line segments both bend up from the given segment, both bend down, or bend in opposite ways). A major question, which I had solved the previous year, was how to handle fixed boundaries and triple junctions. A second potential problem, that of changing topology due to portions of curves meeting and annihilating, was fairly easily solved and programmed.

The papers and videos referred to above are:

(i) Jean E. Taylor, *Motion of Curves by Crystalline Curvature, Including Triple Junctions and Boundary Points*, to appear in the Proceedings of the AMS Summer Institute on Differential Geometry, held in July 1990. This is the definitive paper.

(ii) Jean E. Taylor, *Motion by Crystalline Curvature*, in Computing Optimal Geometries (Jean E. Taylor, ed.), AMS Selected Lectures in Mathematics, 1991, 63-65 plus 7 1/2 minute video. (This publication has both a written and a video component).

(ii) Jean E. Taylor, *Crystalline Geometric Crystal Growth*, in Workshop on Theoretical and Numerical Aspects of Geometric Variational Problems, Proc. of the Centre for Mathematics and its Applications, Australian National University 26 (1991), 231-234.

2. Writing two large overview papers, to be published in the July 1992 issue of Acta Metallurgica. The first paper, joint with John Cahn and Carol Handwerker, surveys nine different mathematical methods for trying to solve the problem of geometric crystal growth, outlining the methods and giving the circumstances in which each performs best. It also surveys all computational methods of which we are aware. My work on this paper involved considerable effort to understand the various methods, such as viscosity solutions of Hamilton-Jacobi equations, with which I was not previously familiar, and to make them intelligible to Cahn and Handwerker in particular and materials scientists in general. The companion paper is a survey of the different ways in which mean curvature and weighted mean curvature can be represented and interpreted, with the emphasis on the non-isotropic cases. John Cahn wrote of it as follows: "This is a difficult paper, and you may want to obtain some help from a mathematician, but it is the clearest exposition of the principles that I know." Full references are:

(i) Jean E. Taylor, John W. Cahn, and Carol A. Handwerker, *Geometric Models of Crystal Growth*, Acta Metall. Mater. 40 (1992), 32 pages in page proof.

(ii) Jean E. Taylor, *Mean Curvature and Weighted Mean Curvature*, Acta Metall. Mater. 40 (1992), 11 pages in page proof.

3. Working out one of the major features of how surfaces move by crystalline curvature, and continuing the preparation of a computer program to do it. In the period since the expiration of the grant, I have worked out what I believe is the remaining major part, programmed it, and made a video and a short paper about it for publication. The detailed paper with proofs is still in the formative stages.

(i) Jean E. Taylor, *Geometric Crystal Growth in 3D via Faceted Interfaces*, in Computational Crystal Growers Workshop (Jean E. Taylor, ed.), Selected Lectures in Mathematics, Amer. Math. Soc. (1992), 3 pages plus a 5 minute video. In press.

(ii) Jean E. Taylor, *Motion of Surfaces by Crystalline Curvature,*, in preparation.

4. Helping to devise a new theoretical variational approach to motion by mean curvature or weighted mean curvature, and establishing rigorously the connection between the crystalline method and the completely variational method. Much of the work and part of the writeup was done during the grant period.

(i) Fred Almgren, Jean E. Taylor, and Lihe Wang, *Curvature Driven Flows,* to appear in SIAM Journal of Control and Optimization. This is the major paper.

(ii) Fred Almgren, Jean E. Taylor, and Lihe Wang, *A variational approach to motion by weighted mean curvature,* in Computational Crystal Growers Workshop (Jean E. Taylor, ed.), Selected Lectures in Mathematics, Amer. Math. Soc. (1992), 4 pages. In press. This is a short expository summary of the above approach.

5. Supervising my graduate student Andrew Roosen in his work applying the crystalline method to dendritic crystal growth and Ostwald ripening by coupling a diffusion field into the driving force. This work has been proceeding in spectacular fashion, and Roosen has obtained a postdoc position at NIST to work with Cahn after he finishes his Ph.D. I wrote one joint paper on this with Roosen, and he has published one additional paper since then.

(i) Andrew Roosen and Jean E. Taylor, *Simulation of crystal growth with facetted interfaces, in Interface Dynamics and Growth,* MRS Symposia Proc. Ser. Vol 237, to appear (12 pages). This paper is a fairly complete description of the algorithm used and a brief description of the theoretical ideas behind it, together with 4 pages of pictures of the output of the program.

(ii) Andrew Roosen, *Simulation of two-dimensional facetted crystal growth in a single diffusion field,* in Computational Crystal Growers Workshop (Jean E. Taylor, ed.), Selected Lectures in Mathematics, Amer. Math. Soc. (1992), 3 pages plus 6 minute video. In press. This is a short expository summary of the above approach, together with a video showing the results of the program under varying conditions leading to dendritic crystal growth or dense branching. It also shows an application to Ostwald ripening with 2000 initial crystals.

6) Finishing the paper *Destabilization of the Tetrahedral Point Junction by Positive Triple Junction Line Energy,* with Frank Morgan. This paper points out that the standard tetrahedral point junction, where four regions meet at a point, is no longer energy-minimising when a junction line energy is included in the total energy along with surface area. Rather, a surface with a line segment along which four surfaces meet is shown to have less total energy. An estimate is made for the length that such a four-fold junction line might be expected have, based on estimates for line junction energy that are given by dislocation energies; this distance is of the order of several atomic dimensions and might therefore be seen in experiments. Brakke's computer program *evolver* was used to compute the figures for the paper and to get better estimates for some of the numbers.

i) Frank Morgan and Jean E. Taylor, *Destabilization of the Tetrahedral Point Junction by Positive Triple Junction Line Energy,* Scripta Met. et Mat. 25 (1991), 1907-1910.

7) Writing the paper *The Motion of Multiple-Phase Junctions under Prescribed Phase-Boundary Velocities.* This paper has still not yet been totally completed, since I have not put it at a very high priority, but it should be finished soon. It shows that the motion of triple junctions can in general uniquely defined, using Huygen's principle of least time,

for three arbitrary normal velocity functions and three arbitrary half lines meeting at a point. This motion can be found by the appropriate use of characteristics, with something like "refraction" of the characteristics when the growth is first through one phase and then another. There are important exceptions: situations where there is no solution, and situations where for certain initial configurations, there is non-uniqueness (although once growth has started using any of the possibilities, it is then unique for all subsequent time). One accomplishment during this grant period was that I found and fixed a problem with part of my description of the least time formulation in this multiple-phase case.

Jean E. Taylor, *The Motion of Multiple-Phase Junctions under Prescribed Phase-Boundary Velocities*, (nearly finished) preprint.

8) Organizing the AMS Special Session on Computing Optimal Geometries with Fred Almgren and Al Marden (held at the AMS meeting in San Francisco, January 1991), and initiating and editing the proceedings of that session as the AMS publication Computing Optimal Geometries, in the series Selected Lectures in Mathematics. A novel feature of this proceedings is that it is a 70 page book together with a 90 minute videotape. The book contains 16 papers and the videotape contains 14 videos.

9) Organizing the Computational Crystal Growers Workshop, held at the Geometry Center Feb. 24-28, 1992. I conceived of and did much of the organisational work during the period of this grant; since then, I have organized a proceedings quite similar to the Computing Optimal Geometries proceedings (it is now in press).

10) I gave a large number of invited talks at a large number of conferences and universities. These include

Frontiers of Science, Irvine, CA Nov. 1990

Materials Research Society fall meeting, Dec. 1990

Mathematical Sciences Research Institute, Berkeley, Jan 1991

AMS winter meeting (1 special session), San Francisco Jan 1991

The Metallurgical Society winter meeting, New Orleans Feb. 1991

Carnegie-Mellon workshop, Pittsburgh, March 1991

Australia: 5 talks under 5 auspices in 3 cites, including an invited hour address at the Australian Math Society annual meeting, June-July 1991

Regional Geometry Institute, South Hadley July 1991

Institute for Theoretical Physics, Aspen, August 1991

AMS regional meeting (2 special sessions), Philadelphia Oct. 1991

U Mass GANG seminar Sept. 1991

Williams College Math Colloquium Sept. 1991

Materials Research Society fall meeting, Boston, December 1991

This grant provided major portions of my support at all of the non-mathematics meetings above.

11) The four papers which I had previously written but which appeared in print during the grant period are:

i) Jean E. Taylor, *On the Global Structure of crystalline Surfaces*, Discrete and Computational Geometry 6 (1991) 225-262.

ii) Jean E. Taylor, *Zonohedra and Generalized Zonohedra*,

Amer. Math Monthly 99 (1992), 108-111.

iii) Jean E. Taylor, *Constructions and Conjectures in Crystalline Nondifferential Geometry*, in Differential Geometry, B. Lawson and K. Tenenblat, eds., Pitman Monographs and Surveys in Pure and Applied Math. 52 (1991), 321-336.

iv) John W. Cahn, Jean E. Taylor, and Carol A. Handwerker, *Evolving crystal forms: Frank's characteristics, revisited*, in Sir Charles Frank OBE, FRS: An eightieth birthday tribute. R.G. Chalmers et al, eds., Adam Hilger, Bristol (1991) 88-118.

Also, a video for which I was one of the authors was published during this grant period, as the video portion of:

(iv) Fred Almgren, *Computing Soap Films and Crystals*, in Computing Optimal Geometries, Jean E. Taylor,
ed., Selected Lectures in Mathematics, Amer. Math. Soc. 1991.